CYCLOHEXANE

CAS Registry Number: 110-82-7

Molecular Formula: C_6H_{12}







"Boat" "Chair"

Cyclohexane is a colorless, flammable, mobile liquid with a pungent odor. It is insoluble in water and soluble in alcohol, acetone, benzene, ethanol, ethyl ether, olive oil, and carbon tetrachloride. Cyclohexane is a non-corrosive liquid and will volatilize quickly. It sublimes between -5 to 5 °C (HSDB, 1993).

Cyclohexane is a typical alicyclic hydrocarbon (Sax, 1987). It may exist in two interconvertible conformations, the boat and the chair. In the chair form, 12 extracyclic bonds fall in two classes. Six of the bonds lie parallel to the main axis of symmetry and are designated as axial, while the other six extend radially outward at +109.5 degree angles to the axis and are designated as equatorial (Merck, 1989).

Physical Properties of Cyclohexane

Synonyms: hexamethylene; hexanaphthene; hexahydrobenzene

Molecular Weight: 84.18
Boiling Point: 807 °C
Melting Point: 6.47 °C

Flash Point: -18 °C (closed cup)

Vapor Density: 2.98 (air = 1)

Vapor Pressure: 97.6 mm Hg at 25 °C
Density/Specific Gravity: 0.779 at 20/4 °C (water = 1)

Log Octanol/Water Partition Coefficient: 3.18 (est)

Conversion Factor: $1 \text{ ppm} = 3.44 \text{ mg/m}^3$

(Howard, 1990; HSDB, 1993; Merck, 1989; Sax, 1987)

SOURCES AND EMISSIONS

A. Sources

Cyclohexane is used for the manufacture of nylon. It is also used as a solvent, oil extractant, paint and varnish remover, in glass substitutes, and in solid fuels (Merck, 1989). Cyclohexane is a component of petroleum, and has been detected in tobacco smoke.

Cyclohexane was registered for use as a pesticide; however as of December 21, 1988, it is no longer registered for pesticidal use in California (DPR, 1996).

The primary stationary sources that have reported emissions of cyclohexane in California are petroleum refining, automotive repair shops, and commercial printing and publishing (ARB, 1997b). Cyclohexane has also been detected but not quantified in motor vehicle exhaust by the Air Resources Board (ARB) (ARB, 1995e).

B. Emissions

The total emissions of cyclohexane from stationary sources in California are estimated to be at least 7,700 pounds per year, based on data reported under the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

Cyclohexane is a natural constituent of crude petroleum. It also occurs naturally as a plant volatile and can be released from volcanoes (HSDB, 1993).

AMBIENT CONCENTRATIONS

No ARB data exist for ambient measurements of cyclohexane.

INDOOR SOURCES AND CONCENTRATIONS

Cyclohexane was measured inside vehicles during the summer of 1988 in Raleigh, North Carolina. In-vehicle concentrations were about 5 times greater than those measured in the ambient air. An average concentration of 1.2 nanograms per cubic meter (ng/m³) and a maximum concentration of 12 ng/m³ were measured (Chan et al., 1991a).

ATMOSPHERIC PERSISTENCE

Cyclohexane exists in the atmosphere in the gas phase, and the dominant tropospheric loss process is reaction with the OH radical. The calculated half-life and lifetime of cyclohexane due to reaction with the OH radical is estimated to be 1.3 days, and 1.9 days, respectively (Atkinson, 1995). The reaction products include cyclohexanone and cyclohexyl nitrate (Atkinson, 1994).

AB 2588 RISK ASSESSMENT INFORMATION

Although cyclohexane is reported as being emitted in California from stationary sources no health values (cancer or non-cancer) are listed in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program Revised 1992 Risk Assessment Guidelines for use in

risk assessments (CAPCOA, 1993).

HEALTH EFFECTS

Probable routes of human exposure to cyclohexane are inhalation, ingestion, and dermal contact.

Non-Cancer: Cyclohexane is mildly irritating to the eyes and mucous membranes at a concentration of 300 ppm (HSDB, 1995; ACGIH, 1992). High vapor concentrations may cause anesthesia. The acute toxicity of cyclohexane is considered extremely low, and no systemic poisonings have been reported in humans.

Cancer: Cyclohexane has not been evaluated for carcinogenicity by the United States Environmental Protection Agency or the International Agency for Research on Cancer (U.S. EPA, 1995a).